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Effects of interfacial heat transfer, surface tension and contact angle on the formation of plasma-sprayed droplets through simulation study

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ABSTRACT

A comprehensive numerical study of the effects of interfacial heat transfer, surface tension (1.8 N/m, 1.647 N/m, 1.35 N/m and temperature-dependent values) and contact angles (60°, 90° and 120°) on the droplet spreading behaviour in the formation of the plasma-sprayed splats was conducted. The evolution of splat morphologies with time was accurately captured using a volume of fluid (VOF) model in a 2-D computational domain. The results show that bubbles form at the time of impact and decrease the heat transfer efficiency at the contact points. During spreading, solidification occurs at the droplet edge before maximum spreading. The rapid growth of the underlying solidified layer induces fluid instabilities for the upper liquid layer, which triggers material jetting. The interfacial heat transfer is the key parameter influencing the droplet cooling process and the final splat morphology. Increasing the substrate preheating temperatures (from 27 °C to 300 °C) delays solidification but increases the potential of substrate melting. A low surface tension (1.35 N/m) readily promotes liquid projections, while the contact angle is of less importance in changing the surface morphologies.

1. Introduction

During plasma spraying, powder particles are injected into the plasma stream, where they experience melting and acceleration. The molten (or semi-molten) droplets impact on the substrate surface, spread and solidify to form splats with different morphologies. The splats serve as the basic block of the bulk coating. Such droplet impingement onto the substrate with small diameter scales, high temperatures and velocities involves complex phenomena such as fluid dynamics, solidification, bubble entrapment and interfacial heat transfer. Because all these characteristics occur in the magnitude of microseconds, it is impossible to clearly reveal the entire impact and spreading process in the formation of splats through experimental methods [1,2]. Therefore, computational fluid dynamics (CFD) simulation provides a good alternative to study droplet impact dynamics. The explicit volume of fluid (VOF) model with small time steps is used to accurately capture the transient liquid-gas interface. This model has been widely used in understanding the impact and spreading characteristics of liquid droplets in the range of micrometre- and millimetre-sized water and tin droplets [3–6] and plasma sprayed micrometre metal/oxide droplets [7–10]. The impact dynamics of millimetre-sized isopropanol with low impact velocities onto the preheated substrates were numerically studied [3]. The predicted droplet spreading morphologies and interfacial temperatures demonstrated a good agreement with experimental observation. Tabbara et al. [4] simulated the spreading behaviour of a 2.2 mm molten tin particle at different impacting velocities based on the VOF and solidification models. The growth of the solidified layer experienced three stages of planar morphology, uneven morphology and wave mixing. Through solving a fixed-grid Eulerian model, the spreading behaviour of the molten droplets, either in the micrometre size [7] or in the millimetre size [5], with interfacial heat transfer and solidification, was successfully simulated using 3-D models. Zheng et al. [8] also used the commercial software ANSYS FLUENT to describe the evolution of contact pressure, velocity and temperature fields and solidification in the formation of plasma-sprayed zirconia splats. With ANSYS CFX software, Tran et al. [9] predicted substrate melting and resolidification when molten Ni droplets flattened on stainless steel, and validated the model with experimental observation. Apart from the VOF method, Oukach et al. [11] modelled the spreading behaviour of molten alumina droplets using the Level Set method to track liquid-gas interface.

The formation of single splats in plasma spraying is dependent on a range of factors, such as the high temperature thermal-physical properties of the powder material, the substrate temperature, the droplet contact angle on the substrate surface and the thermal contact resistance along the splat-substrate interface. Through mathematical modelling, Wan et al. [12] found that the surface tension and contact angle were negligible in changing splat spreading diameters during plasma spraying. The substrate preheating conditions and interfacial thermal contact resistance were found to be the key factors influencing droplet spreading diameters, by means of influencing the solidification process. Unfortunately, the instantaneous splat morphology and solidification process were not demonstrated in detail. A clear display is important for understanding how the solidification behaviour influences liquid

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Nomenclature

General symbols

D_0	Droplet diameter before impact
V_0	droplet velocity before impact
t	time
v	velocity
g	gravitational acceleration
k	thermal conductivity
P	pressure
T	temperature
D	droplet spreading diameter
H	total enthalpy
h	sensible enthalpy
ΔH	latent heat
S	solidification parameter
L	latent heat of the liquid phase
x, y, z	coordinate
s	thickness of the solidified layer
n	the surface normal at the interface
C_p	specific heat
A_{mush}	mushy zone constant
$\vec{S}_m$	source term
F_{vol}	volume surface tension force

Greek symbols

α	volume fraction of fluid
ρ	density
μ	viscosity
σ	surface tension
β	liquid fraction
ξ_m	maximum flattening ratio
θ	liquid-solid contact angle
κ	surface curvature

Dimensionless numbers

Co	Courant number$(=vdt/dx)$
We	Weber number$(=\rho {V_0}^2 D_0/\sigma)$
Re	Reynolds number $(=\rho V_0 D_0/\mu)$
s^*	thickness of solidified layer$(=s/D_0)$
Ma	Marangoni number$(=\rho C_p D\lvert d\sigma/dT\rvert \Delta T/2\mu k)$

Subscript symbols

l	liquid
g	gas
w	wall

flowability. Nevertheless, the contact angles were found to be dominant in determining the spreading dynamics without considering the solidification process especially in the case of millimetre-sized liquid droplet [13,14]. More work should be conducted on understanding the role of contact angles on droplet spreading when taking into account the solidification.

Many research groups have focused on studying the splat formation of nickel powder [2,7]. Therefore, nickel material was selected in the simulation for consistently studying droplet spreading behaviour, which may give more informative understanding. Moreover, chromium element as the active element and was found to improve static wetting behaviour of droplets [15]. Our previous experimental study showed that droplet fragmentation was suppressed for Ni20Cr splats compared to Ni splats, and more disk shapes were observed for Ni20Cr material [16]. It has been found that one of the main differences between the high temperature thermophysical properties for Ni and Ni20Cr was the liquid surface tension, which was correlated with the droplet contact angles and wettability. However, it is still unclear whether the formation of more Ni20Cr disk splats results from the difference in surface tension values, or other effects such as interfacial reactions and dynamic wetting with the addition of Cr element. Therefore, it is important to verify the role of contact angle, surface tension and interfacial heat transfer on droplet spreading dynamics in plasma-sprayed splat formation.

In this paper, the behaviour of droplet impact, spreading and solidification was comprehensively studied through CFD simulation. Through accurately demonstrating the time-dependent spreading process and solidification behaviour by simulation, the influence of interfacial heat transfer (consisting of substrate preheating and interfacial thermal contact resistance (TCR)), droplet surface tension and contact angles on droplet spreading was investigated. It should be noted that in this paper the scope is constrained to understanding the droplet impact onto the substrate where there was no surface adsorbents/moisture evaporation. Splat fragmentation induced by the evaporation of surface adsorbents/moisture was not studied numerically.

2. Numerical models

2.1. Computational domain and meshing

The commercial software ANSYS FLUENT 16.0 [17] was used to model the droplet impact and spreading dynamics. A molten Ni droplet of 54 μm diameter with an initial temperature of 2100 K was simulated to impact onto a stainless steel substrate with an initial velocity of 100 m/s. The high temperature thermophysical properties of the Ni droplet and the stainless steel substrate are summarized in Table 1. Three different values of surface tension were used in this paper for understanding its effect on droplet spreading. The value of 1.8 N/m represents the Ni surface tension at melting point (1728 K), while the value of 1.647 N/m represents the Ni surface tension at initial impact temperature (2100 K). The value of 1.35 N/m represents a surface tension comparable with Ni20Cr material at its melting point (more information can be found in Section 3.3). A two dimensional (2D) axisymmetric domain was used in the simulation where the size of air domain was 320 μm × 90 μm, large enough to decrease the backward flow to the boundaries. The dimension of the substrate domain was 320 μm × 25 μm (width X and height Y). Detailed boundary conditions are presented in Fig. 1. When the liquid droplet flowed over the substrate surface, a non-slip wall boundary condition was utilized. This condition assumed that there was no relative velocity between the fluid and stationary substrate surface at the contact line. In reality the contact line would experience slip during droplet spreading. So the definition of a slip length was proposed, considering the velocity gradient at the triple line, to avoid the singularity [18]. Nevertheless, this length scale was much smaller than the grid spacing in the numerical studies [19,20]. Thus, the simplest assumption of a non-slip wall condition was acceptable to predict droplet spreading behaviour. Because of the difficulties in photographing the droplet spreading process, the dynamic contact angles (DCA) cannot be measured along the contact line. Therefore, the equilibrium static contact angle (SCA) was used in the present paper [5]. Qualitatively, the predictions of droplet spreading ratios of DCA and SCA were in a good agreement [6,21].

The meshing quadrilateral element numbers were fixed with 56,000 elements for the substrate domain and 705,600 elements for the air domain. The smallest grid in the air domain was 0.14 μm to accurately capture the droplet-air interface motion. An extensive grid independence test was conducted to confirm that the meshing scheme was sufficiently fine to capture the droplet spreading diameter and the droplet-air interface. In the testing study, three different grid sizes were selected, yielding a minimum cell length of 0.2 μm (400,000 cells in total), 0.14 μm (761,600 cells) and 0.11 μm (1,238,400 cells). The meshing algorithm used in this paper (grid size 0.14 μm) was sufficiently fine to capture